Design of an absorption tower for a laboratory scale CO_2 capture plant

Valeria Román Restrepo[a] , Michel Alejandra Herrera Meneses[a]

Santiago Builes Toro[b]

[a] *Student of Process Engineering , EAFIT University, Medellín, Colombia*

[b] *Professor, Advisor of graduation project, Process Engineering Department, EAFIT University, Medellín, Colombia*

Abstract

Carbon dioxide (CO_2) is the main greenhouse gas in the earth's atmosphere. The current concentration levels of CO_2 in the atmosphere contribute to generate irreversible changes in the climate, sea level and the environment. Due to the highly industrialized economy, for today's society it will not be possible, in the mid-term, to stop these CO_2 emissions without serious economic and social consequences. Therefore, it is necessary to implement several strategies to reduce CO_2 emissions, for instance integrated CO_2 capture systems that are efficient and economically viable. Strategies such as carbon capture and storage can used to reduce the impact of CO_2 emissions on the global climate to an acceptable level.

Reactive absorption with aqueous solutions of amines in an absorber/stripper loop is the most mature technology for CO_2 capture from existing plants. Therefore, it is proposed to design an absorption tower at laboratory scale in stainless-steel due to its stability and resistance to corrosion for the capture of CO_2 using monoethanolamine. This requires the assessment of the best model for describing an absorption tower at laboratory scale by comparing different models and simulations programs to determine the most appropriate one for design at laboratory scale. The model implemented in Python absorption tower design was chosen over the commercial simulators, resulting in a 10 mm Raschig ceramic ring packing, a CO_2 removal rate of 80%, an internal diameter of 21.7 mm and a packing height of 400 mm.

1. Introduction

Climate change caused mainly by manmade emissions of greenhouse gases (GHG) has become a major issue of the 21st century [1]. These emissions affect our climate, increase the sea levels, and threaten the environment [1]. Moreover, human activities, such as the use of fossil fuels and deforestation, have considerably altered the amount of carbon stored in the geosphere and have perturbed the fluxes of carbon in the biosphere [2]. Fossil fuels have and continue to play a dominant role in global energy systems [3]. Combustion of hydrocarbons has negative environmental impacts, such as large emissions of air pollutants, CO_2, and other greenhouse gases [3]. It should be noted that carbon dioxide emissions are a considerable contributor to the gradual increase in global average temperature seen in the last few decades [4]. The natural greenhouse effect, which makes life possible on earth acting as long-wave radiation trap preventing heat from escaping earth, has gradually increased due to the increase in GHG concentration. Additionally, the grow of CO_2 partial pressure in the atmosphere contributes to the rise of natural rainfall acidity since carbon dioxide dissolves in rain drops into carbonic acid [5].

The Paris Agreement has set a target of limiting the average temperature increase to 2.0 °C above pre-industrial levels [6], to prevent global warming from exceeding these 2°C, the net GHG emissions need to be close to

zero or even negative [6]. Therefore, achieving this target requires improving energy efficiency [7], promoting energy conservation [8] and developing technologies for the capture and storage of CO_2 [1].

There are several carbon capture technologies available, such as: absorption [9], adsorption [10], cryogenic distillation [11] and membranes [11]. The most mature method for CO_2 removal is absorption in an amine-based solvent followed by desorption [12]. The most used amine for CO_2 removal is monoethanolamine (MEA). In the MEA-based CO_2 absorption process with a 30%-wt solution of MEA, the flue gas enters the absorber at the bottom and flows upwards while the solvent solution flows downwards, forming a counter flow [13], part of CO_2 in the flue gas is absorbed into the amine solution [14]. Finally, the solution with absorbed CO_2, is pumped to the stripper column to recover the CO_2 and reuse the amine [14].

The main limitation hindering the widespread adoption of this technology for reducing CO_2 emissions is the reported energy penalty which is within a range of 0.37 - 0.50 MWh/(tonne of captured CO_2) [15], which decreases the overall efficiency of the plant due to process steam being used to fulfill the stripping task instead of energy production [16].

It is necessary to design correctly and accurately the absorption equipment at laboratory scale. Absorbers are used to a great extent in industrial complexes and plants to separate and purify gaseous streams, to recover valuable products and chemicals, as well as for pollution control [17]. The most common absorber types employed in industry are plate columns, packed towers, venturi cleaning towers and spray chambers [17]. Packed towers are widely used for gas-liquid absorption operations and, to a limited extent, for distillations [17]. The design of a packed absorption tower includes the determination of geometrical parameters such as tower diameter (D) and packing height (Z), as well as some other mass-transfer and operational variables such as convective mass-transfer, as well as overall mass-transfer coefficient [17]. A well-designed packed tower must be integrated with the other process equipment [17]. A proper absorption tower design seeks a low pressure drop, small capital and operating costs, and high removal efficiencies [17]. Therefore, this project aims to redesign a glass absorption tower available at the research incubator DPI at Universidad EAFIT, seeking a proper design for the removal of CO_2. For this purpose, the simulation programs Aspen Plus and Aspen HYSYS are used, as well as an implementation of the absorption algorithm in Python, this gives us the possibility to understand the process behavior under various process conditions and help us to identify optimum conditions [18]. Aspen HYSYS and Aspen Plus are two simulation programs that are widely used in the industry for steady state process simulations and calculations of equilibrium data for various gas liquid mixtures [18]. On the other hand, in Python different libraries are used to develop the mathematical equations constituting the process model. The idea is to choose the best model based on a ratio of CO_2 removal efficiency and the associated equipment costs.

The main goal of the present work is to redesign and choose the simulation program that best characterizes the sizing of an absorption tower at laboratory scale, considering experimental data available in the literature This is part of ongoing efforts of research incubator DPI at Universidad EAFIT for the continuous operation of a laboratory plant for the capture of CO_2. The sizing and design of the absorber assumed that the solvent in the process was a 30%-wt solution of MEA due to the large availability of data for the equilibrium and mass transfer of this solution and carbon dioxide.

2. Materials and methods

2.1. Inlet conditions

The data for the design of the absorption tower in the Python simulation program were taken from an experimental study [19], which uses 30%-wt solutions of MEA at various loadings. This was used as the initial input for sizing the absorption tower according to the desired output conditions [19].

For carbon dioxide, the following inlet conditions were used: a gas flow rate of 5 L/min, a gas fraction of 10% mol CO_2, an inlet temperature of 25°C and an absolute pressure of 125.64 kPa [19]. For aqueous MEA, the

following conditions were used: a liquid flow rate of 0.1 L/min, a liquid MEA fraction of 11.2 % mol (30%-wt) and an inlet temperature of 50°C [19].

These conditions were also used in Aspen Plus V11 and Aspen HYSYS V11 simulations of the CO_2 absorption tower with MEA. The Electrolyte-NRTL activity coefficient model for liquid and PC-SAFT equation of state were used in Aspen Plus for the thermodynamic properties [20] this model was validated by Zhang et al. [21] against experimental data of the MEA–H_2O–CO_2 system with temperature up to 443 K, pressure up to 20 MPa, MEA concentration up to 40%-wt and CO_2 loading up to 1.33 [21]. The Acid Gas Chemical Solvents package which was validated by Amundsen [22] for 30%- wt MEA, was used in Aspen HYSYS as a model for the calculation of the physical properties. This model helps with the reactions and chemistry using the underlying thermodynamics and calculation models [23].

Due to the need to enter all the inlet conditions and the compositions of the interacting species, unlike the design carried out in Phyton, in Aspen Plus and Aspen HYSYS the inlet compositions for the flue gas were taken from a natural gas stream [24] as shown in *table 1*. In addition, it was necessary to use approximate values to measure the diameter and packing height of the tower at laboratory scale to facilitate the convergence of the model towards this desired scale. The inlet diameter used of 24.4 mm was taken from the conceptual design in Python, and the initial inlet packed height of 600 mm was taken from the corrected simulation of Mejia et al. [25]. The last value was further adjusted to obtain a given removal percentage in both simulators.

Table 1. *Flue gas compositions used for Aspen Plus and Aspen HSYYS simulations.*

Substance	**Mass fraction**
N_2	0.743
O_2	0.101
H_2O	0.071
CO_2	0.085

Since MEA has corrosive properties and the local providers offer is limited, stainless steel SS304 was selected as the construction material, due to its high strength, excellent corrosion resistance and excellent formability [27].

2.3. Evaluate the different simulation programs used in the design of the absorption tower.

Python simulation

The algorithm designed in Python was made using the numpy library, which specializes in numerical computation and data analysis, especially for large volume data. Math- contains a wide variety of mathematical functions. Other libraries such as Pandas, which allows the manipulation and analysis of data, and matplotlib.pyplot, which allows the creation of graphs, were also used. Each of the equations was developed based on the literature [26,17]. Some parameters were varied during the different simulations performed with the program, such as input and output conditions to see how the results responded. *Figure 1* shows an example of how Python code development looks like.

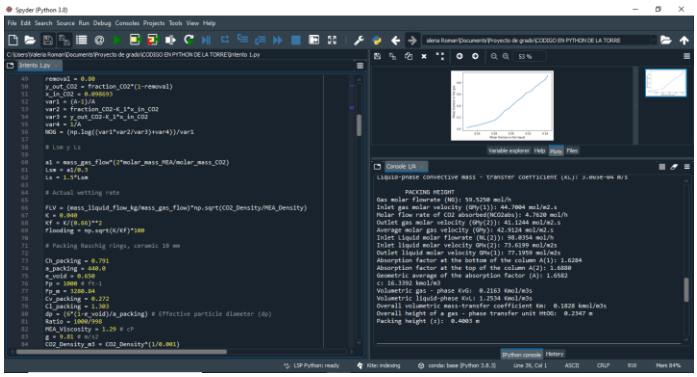

Figure 1. *Sample image of the integrated development environment used for the absorption tower design algorithm in Python, along with the CO_2 equilibrium plot and some relevant results.*

When calculating the internal diameter of the tower, the resulting value should be approximated to a standard pipe size, and afterwards checking the percentage of flooding once the standard diameter is used.

Regarding the design of the equipment, the following data must be considered: (i) Equilibrium data of CO_2 in liquid and gas phase, (ii) gas and liquid flow rates (L/G), (iii) the changes in the solute concentration to form the operation line and (iv) individual and overall volumetric mass transfer coefficients.

Since the absorption tower in this case is a packed tower, in our case we will use 10 mm Raschig ceramic rings, because they provide a good contact between the liquid and the gas; are useful for resisting corrosion at elevated temperatures, where plastic may not be suitable; and they have a good wettability [17]. Raschig ceramic rings with the nominal diameter indicated above are chosen because they are the second smallest size available [26] and fit the sizing of the absorption tower at laboratory scale.

A flowchart of the absorption tower design methodology in Python is illustrated in *figure 2*. It is a modified version of the absorption tower design methodology developed by Thakore et al. [26].

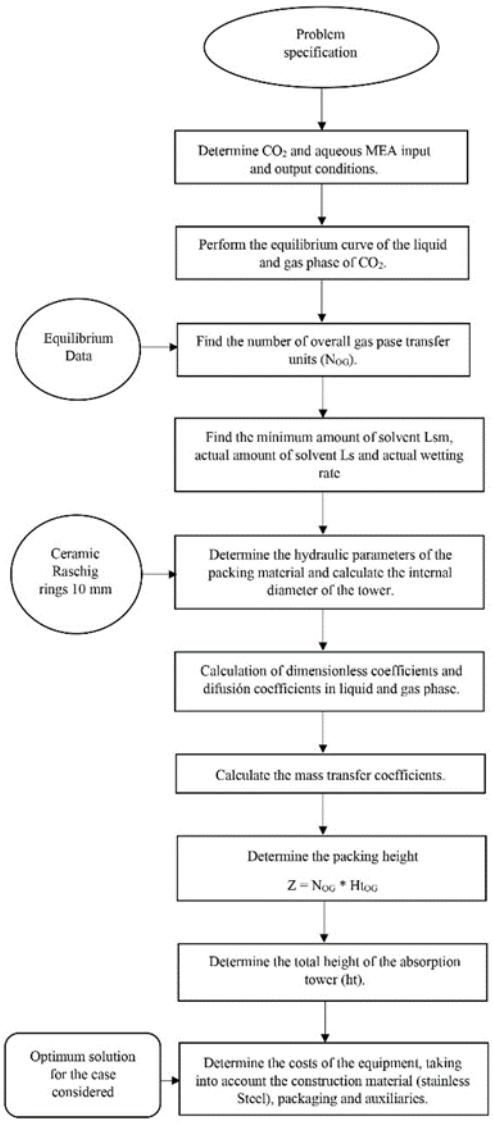

Figure 2*. Schematic of the absorption tower design methodology as implemented in Python.*

Determining the packed column height necessary for the mass transfer of CO_2 from the gas phase to the liquid phase requires accurate predictions of the mass transfer coefficients [28]. Different separation equipment can be used for the CO_2 capture process, including columns with tray, spray, packing types and membrane contactors [28]. Of all the above-mentioned separation devices, the most complicated ones to design are the packed columns due to the complex relationship between the mass/heat transfer, hydromechanics, and thermodynamics [28].

Aspen Plus simulation

The Aspen Plus simulation was carried out with the *rate-based* multistage separation model which assume that separation is caused by mass transfer between the contacting phases [20], as opposed to equilibrium-stage models that assume each theoretical stage with well-mixed vapor phase and liquid phase and that these two phases are in phase equilibrium which each other [20]. The rate-based model considers the heat transfer coefficients for the calculations; therefore, the geometry and size of the equipment are required for the

calculation [25]. This allows sizing the tower through the simulation results (and not heuristics) based on desired operative conditions [25] and inlet streams.

The number of stage specification was taken from Zhang et al [20] rate-based model who obtained 84% of CO_2 removal in their experimental absorber. Five discretization points were chosen for the liquid phase into the rate-based setup, this option allows to rigorously model the mass transfer resistance and the CO_2 absorption reactions taking place in the liquid film [20].

A removal rate of 80% for CO_2 was defined for the simulation considering the number of stages and the discretization rate for the liquid phase of the pilot plant of Zhang et al [20], where the absorption percentage varied between 80-87%. In addition, the absorption result of the Python design was considered, to finally establish a CO_2 removal of 80%.

Since Aspen Plus is purely a modular sequential simulator the removal percentage was adjusted indirectly using the Design Spec. Moreover, the tower diameter was adjusted according to the flood factor, following the heuristic approach that a flooding condition should be below 80% for packed columns [25,29], and the pressure drop of the system, restricted to between 200 and 400 Pa/m, controlled with the hydraulics plots. The packed height of the tower was then adjusted based on the removal specification of CO_2. The final dimensions were obtained when 80% of the inlet CO_2 was captured with a flood percentage lower than 80% and the pressure drop within the ranges of consideration.

The packing height for the tower was obtained as the result of an iterative process where the height was adjusted range between 0.6 and 2 m until the target removal was achieved subject to the process restrictions. This range was chosen considering that the flow simulators work with larger scales due to the configuration of the system, but also, considering that the height of the tower packing should not exceed 2m because it would be greater than expected from a laboratory scale.

For the packing specification, 13mm Raschig rings were chosen, instead of the 10 mm ones used in Python, because it is the smallest offering in Aspen Plus for this type of packing. This means that the program structure does not consider the necessary configurations for models with laboratory scale dimensions.

The calculation process in Aspen Plus is summarized in a flowchart in *figure 3*. This flowchart is different from the flowchart used in Python because Python is a programming language where different libraries are used for each area of emphasis or need and all the data and equations of the design must be entered, while Aspen Plus, like Aspen HYSYS are flow simulators, where the equations of state, thermodynamic packages and the design equations of the different equipment are within the configuration of the program, the essential thing for its operation is to enter all the conditions input (temperature, pressure, compositions, flows and dimensions).

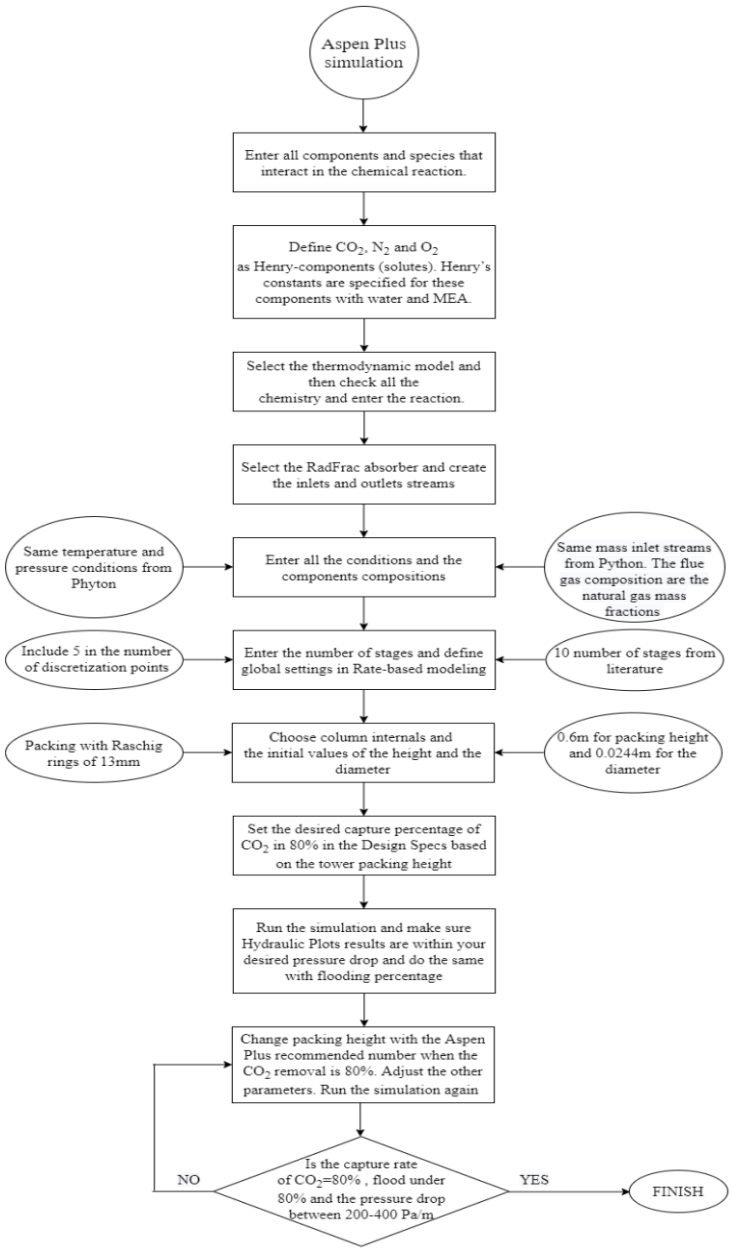

Figure 3. *Schematic flowchart of the design methodology of the absorption tower implemented in Aspen Plus.*

Aspen HYSYS simulation

The absorption column model in Aspen HYSYS has a default set of convergence criteria, and a default set of calculation parameters based on specified inlet streams which must be known prior to the calculation [24]. Unlike Aspen Plus with the rate-based model, the "Efficiency" option was chosen as a type of calculation of the column in Aspen HYSYS [23]. The quicker "Efficiency" calculation type is the one most used thanks to the accuracy and ease of use [23]. It is a highly rigorous method that uses rate-based calculations in the background to calculate stage efficiencies of H_2S and CO_2, and then uses these values to solve the column. Also, in column descriptions the column was specified with the Rating model, which means that the geometry will be a result of the simulation however these results will not automatically update when simulation results change, and the user must manually input changes to the geometry [29]. This is necessary to choose the packing type.

The same inputs and sizing conditions used in Aspen Plus were used for the Aspen HYSYS simulation of the tower. Although Aspen HYSYS has the option to put the 10 mm Raschig rings packing, like the ones used in Phyton, the 13 mm Raschig rings were chosen to aid in the comparison between the flowsheet programs. Moreover, it is necessary to use the same measurement so that there are no large changes in the pressure drop and in the height of the packing because the type and dimension of this affects the flow cross section and therefore, there could be changes in the final height of the tower packing.

The packing height for the tower was again obtained by fixing the 80% removal of CO_2 as a process restriction in the *Adjust manager*. The CO_2 flow at the outlet of the sweet gas was established as a fixed variable and a height objective was established between 0.6m and the final value of the height of the Aspen Plus packing where the required removal percentage was achieved. This objective of 0.6 m for the packing of the tower was established considering the corrected simulation of Mejia et al [25] where this value was found for a pilot scale absorption tower but with its correction factor. This value is lower than a pilot scale, considering the examples from the literature such as Zhang et al [20] where an 11.1 m tower was obtained on a pilot scale, therefore, the value of 0.6m was an initial value correctly chosen for the convergence of the simulator towards a laboratory scale. The calculation process in Aspen HYSYS is summarized in a flowchart in *figure 4*.

Figure 4. *Schematic flowchart of the design methodology of the absorption tower implemented in Aspen HYSYS.*

Figure 5 shows a sample flowsheet view of the parameters used for the simulation in the flowsheet programs (Aspen Plus and Aspen HYSYS).

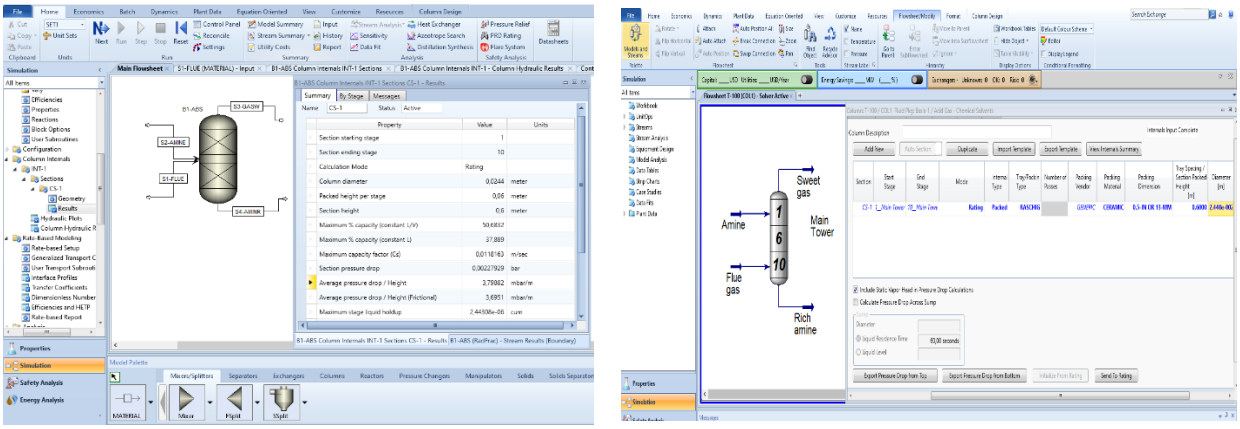

Figure 5. *Flowsheet programs view of the absorption tower design.* Left: a view of the Aspen Plus simulator, with the RadFrac-type absorption tower. Right: Aspen HYSYS absorption tower and the window for the tower packing specification.

2.4. Sizing- Analysis of the absorption tower

The equilibrium plot of CO_2-MEA-WATER in liquid and gas phase for carbon dioxide was constructed from CO_2 solubility data in 30%-wt MEA as function of CO_2 partial pressure from the literature [30]. As can be seen in *figure 6* the original data was transformed to obtain the equilibrium curve. The chemical equilibrium is given when the concentration of CO_2 in liquid and vapor phase did not change and likewise no physical changes are observed as time passes, with the slope of the graph we can get the equilibrium constant.

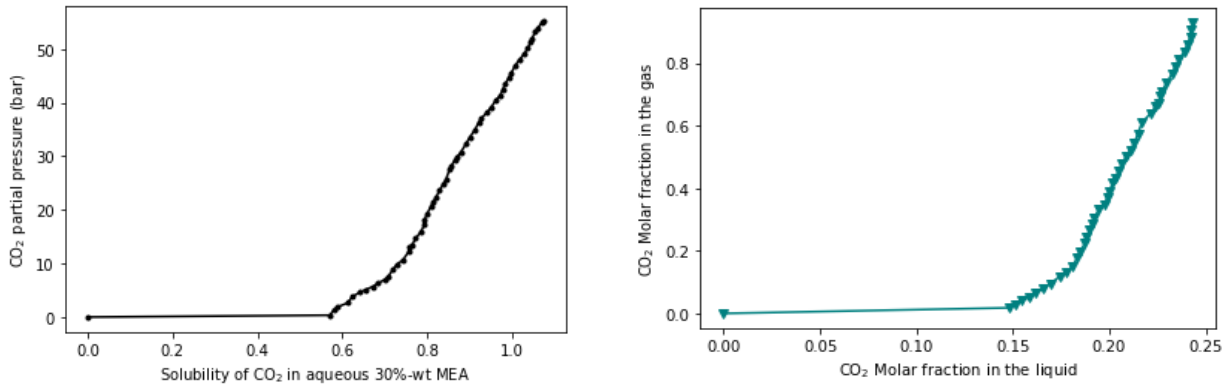

Figure 6. *On the left side is a graph of CO_2 solubility in 30wt % aqueous MEA [30] taken from the literature and on the right side is a graph of CO_2 liquid and gas phase equilibrium data.*

The slope of the equilibrium curve corresponds to the equilibrium constant (K), which can be used to calculate the number of overall gas phase transfer units (N_{OG}). The parameters y_{in} and y_{out} refer to the mole fraction of CO_2 in the gas phase at the inlet and outlet, respectively. On the other hand, x_{in} refer to the mole fraction of CO_2 in the liquid phase at the inlet.

$$N_{OG} = \frac{\ln\left\{\left[\frac{A-1}{A}\right]\left[\frac{y_{in} - Kx_{in}}{y_{out} - Kx_{in}}\right] + \left(\frac{1}{A}\right)\right\}}{(A-1)/A} \quad (1)$$

Where *A* corresponds to:

$$A = \frac{L}{KV} \quad (2)$$

In *equation 2*, the L parameter corresponds to the molar flux of the liquid and V refers to the molar flux in the vapor. To calculate the minimum amount of solvent L_{sm}, the following chemical reaction must be considered:

$$CO_2^+ + 2MEA \rightleftharpoons MEACOO^- + MEAH^+ \quad (3)$$

And then to find the actual amount of solvent L_s, we used the following relation:

$$L_S = 1.5L_{sm} \quad (4)$$

To find the tower diameter, at first the following factor (F_{LG}) was calculated according to *equation 5*. Parameter L_w refers to mass velocity of liquid, G_w to mass velocity of gas, ρ_G to the density of gas and ρ_L to the density of liquid.

$$F_{LG} = \frac{L_w}{G_w}\sqrt{\frac{\rho_G}{\rho_L}} \quad (5)$$

Using the generalized flooding and pressure-drop correlation chart for packings [26], the corresponding value of K_{SLEC} at flooding (K_f) is determined. Also, we need to consider the following relation:

$$K_{SLEC} = (0.66)^2 K_F \quad (6)$$

All hydraulic parameters must be extracted from the literature [26] for the packing material, which corresponds to 10 mm ceramic Raschig rings. These parameters are: Nominal size, packing factor (Fp), void space percentage, hydraulic factor (Ch), mass-transfer surface per unit volume (a) and mass transfer factors (Cv, Cl).

The mass velocity of the gas through the tower can be calculated using *equation 7*. Parameter g refers to the gravitational acceleration, F_P to the packing factor, ψ to the ratio of density of water to density of liquid, μ_L to the viscosity of liquid, K_{SLEC} to the function of velocity of gas through tower, and ρ_G-ρ_L to density of gas and liquid.

$$G_w = \left(\frac{K_{SLEC} * \rho_G * \rho_L * g}{Fp * \psi * \mu L^{0.2}}\right)^{1/2} \quad (7)$$

The internal diameter of the tower was calculated according to *equation 8*. Parameter G_{1w} refers to feed gas flow rate, D to diameter of the tower and G_w to mass velocity of gas.

$$\frac{\pi}{4} * Di^2 = \frac{G_{1w}}{G_w} \quad (8)$$

Before calculating the diffusion coefficients, the following parameters must be calculated: Gas-phase Reynolds number (Re_G), liquid mass velocity (G_L), the liquid velocity (v_L), liquid-phase Reynolds number (Re_L), liquid-phase Froude number (Fr_L), the ratio ah/a, the effective specific surface area of packing (ah) and finally the liquid holdup (h_L) [17]. Once this is done, the diffusion coefficients are calculated. To calculate the gas-phase diffusion coefficient, *equation 9* is used. Parameter M_{AB} refers to the interaction between CO_2 and MEA, T to temperature, P to pressure, σ_{AB} to collision diameter and Ω_D to diffusion collision integral.

$$D_G = \frac{\left[3.03-\left(\frac{0.98}{MAB^{1/2}}\right)\right]*(10^{-3})*(T^{3/2})}{P*MAB^{1/2}*\sigma AB^2*\Omega D} * 0.0001 \quad (9)$$

To determine the liquid – phase diffusion coefficient in binary systems, *equation 10* is used. Parameter V_{MEA} refers to molar volume of the solution of monoethanolamine and μ_W to viscosity of water.

$$D_L = \frac{1.25x10^{-8}*(VMEA^{-0.19}-0.292)*T^{1.52}*\mu W^n}{10000} \quad (10)$$

The gas-phase convective mass-transfer coefficient (k_G) was calculated according to *equation 11*. Parameter C_V refers to mass transfer factor, a_{SA} to mass-transfer surface area per unit volume, ε to packing porosity or void fraction, K_W to wall factor and Sc_G to the Schmidt number for gas phase.

$$k_G = 0.1304*C_V * \left[\frac{D_G*P}{R*T}\right] * \left(\frac{a_{SA}}{[\varepsilon*(\varepsilon-h_L)]^{0.5}}\right) * \left[\frac{Re_G}{K_W}\right]^{3/4} * ScG^{2/3} \quad (11)$$

The liquid – phase convective mass-transfer coefficient (k_L) was calculated according to *equation 12*. Parameter C_L refers to mass transfer factor.

$$k_L = 0.757*C_L * \left[\frac{D_L*a_{SA}*v_L}{\varepsilon*h_L}\right]^{0.5} \quad (12)$$

Prior to determine the overall height of a gas-phase transfer unit (HTU), it will be necessary to calculate several parameters. HTU was calculated according to *equation 13*. Parameter G_{My} refers to average molar gas velocity and K_m to overall volumetric mass-transfer coefficient.

$$H_{tOG} = \frac{G_{My}}{K_m} \quad (13)$$

Finally, the packing height was calculated according to *equation 14*.

$$Z = N_{OG} * H_{tOG} \quad (14)$$

2.6. Mechanical design of the absorption tower

The mechanical design was carried out considering the dimensions of the packed tower in QCAD. Besides the packing section and diameter calculated in the process design software it was necessary to determine the height of the upper and lower sections of the tower, establish a thickness for the packing supports, choose a lid for the tower, establish a measurement for the diameter of the pipes and select the threaded coupling for the union between pipelines and find the right liquid distributor because this is a key element of the packed column and packing efficiency. This last item was chosen according to the options offered by the commercial distributor.

To calculate the height of the upper and lower part of the tower, it was necessary to make a relationship between the height of the packing and the height of the upper part with the data from Castro [31] and those obtained in the present work.

The packing hold-down and packing support were taken from Castro [31], who recommends that a support of at least 5mm in a laboratory scale absorption tower will be sufficient to support the tower packing.

The lid of the container, located in the upper part of the tower, was chosen with a hemispherical design because it does not have a dimensional limit for its manufacture [32]. The same internal diameter of the tower was used for the lid.

For the selection of the diameter of the pipes used for building the tower, the height of the packing and its diameter were also considered. Having a laboratory scale absorption tower requires that the dimensions be suitable for the flow rate, but that in turn, these dimensions comply with the standards of the materials that can be purchased commercially. That is why pipes with a ½ in nominal diameter, that is, 21.3 mm in outside diameter, were chosen.

The flange is a metallic piece that joins two components of a piping system, usually by means of screws [32]. It had to be considered: for pipe diameters of 1 ¼ in diameter and smaller be installed using 3000 and 6000 lb/in^2 stainless steel threaded couplings. Larger pipe diameters will require flanges [32].

2.5. Absorption tower cost estimation

An excel spreadsheet was programmed to perform the cost calculations for the absorption tower using the data reported in Python and based on the mechanical sizing done for the equipment. This was achieved based on the following equations [33, 34]:

Equation 15 allows to calculate the purchase cost of the packing for the equipment, considering the required surface area of packing.

$$\text{Packing purchase cost} = \text{Required packing surface area} * \left(7.31 + \frac{203.05}{a}\right) \quad (15)$$

The cost of the column has been computed using the *equation 16*. Where the parameter H_{total} denotes the total height of the tower. F_{mat} represents a correction to consider for the cost of the material, in our case it has a value of 1.7 and p represents absolute pressure.

$$C_{Col} = 583.6 * D^{0.675} * H_{total} * F_{mat} * \left(\frac{p*14.5}{50}\right)^{0.44} \quad (16)$$

To calculate the capital expenditure (CAPEX) which refers to expenditures on capital equipment and results in profits that guarantee and measure its growth, the *equation 17* is used to find this value.

$$\text{CAPEX} = \text{Packing purchase cost} + C_{Col} \quad (17)$$

To calculate the operating costs of the absorption tower, the pump must be considered since energy costs are incurred during the process and should also include the purchase cost of the MEA.

3. Results and discussion

The design of the lab – scale packed absorption tower was carried out in Aspen Plus, Aspen HYSYS and Python, to compare among the programs and select the most reliable results for the laboratory scale design. 30%- wt aqueous MEA was used as solvent, the input conditions of the components, the nominal diameter of the packing and the percentage of CO_2 removal were varied to see in what proportion CO_2 is absorbed at the end of the design. It was observed that if the solvent rate is very small, the removal capacity is not sufficient unless the near-rich solution is regenerated with a very low CO_2 lean load [19]. On the contrary, if the solvent rate is very high, a lot of energy is required to overcome the temperature difference between the absorber and the stripper [19].

Design of the absorption tower in Python

After simulating the design of the absorption tower in Python, the main parameters shown in table 2 were obtained, which lead us to determine the internal diameter, the height of the packing and the height of the tower.

***Table 2**. Main results of the packed absorption tower design in the Python simulation program*

Parameter	Value	Units
Amount of CO_2 absorbed (mCO_2abs)	0.2096	kg/h
Amount of solvent liquid exiting the column	6.1976	kg/h
K	0.022	
L/V	6.4475	
A	1.6582	
N_{OG}	1.7054	
% Flooding	66%	
Mass velocity of gas	0.5025	kg/(m^2s)
Actual wetting rate	2703.4274	m3/(h.m^2)
Flow parameter	0.4378	
Pressure drop parameter under flooding conditions (Yflood)	0.0653	
Coefficient at flooding conditions (Csflood)	0.0113	m/s
Gas velocity at flooding conditions (Vgflood)	0.2381	m/s
Gas velocity (vg)	0.1572	m/s
Liquid mass velocity (G_L)	4.6541	kg/m^2.s
Liquid velocity (vL)	0.0047	m/s
Inside diameter of tower	0.8544	in
% CO_2 removal	80%	
Packing height (z)	0.4003	m

For the inlet conditions, the volumetric gas flow rate was 300 L/h, the gas temperature was 25°C and the CO_2 mole fraction at the inlet was 0.1. With respect to the solvent, a volumetric liquid flow rate of 6 L/h was taken, the temperature for the liquid was 50°C and the mole fraction of aqueous MEA at the inlet was 0.112. These values were taken from the literature [19] to develop the simulation algorithm in Python.

As shown in *table 2* for the internal diameter, a value of 0.8544 in (21.7017 mm) is obtained, which is consistent with the expected values for a laboratory scale equipment. Given the diameter of the tower, a standard pipe should be found that fits this value. The pipe most in line with the design of the absorption tower is one with ½

in in nominal diameter, that is 0.8386 in (21.3004 mm) for the outside diameter. Another aspect to be considered is the packing height for which a value of 400 mm is obtained as shown in *table 2*.

Due to the nature of the CO_2 capture process and the associated complexity, it is necessary to study the impact of individual variables to understand their implications when systematic changes occur. Therefore, the impact of the critical variables of the process is analyzed below.

In *figure 7*, as the volumetric gas flow rate increases, the packing height and diameter increase in a similar proportion.

If we double the gas flow from 100 to 200, the diameter varies by 0.2043 in, and the packing height differs by 1.8662 in. On the other hand, if we double the flow from 200 to 400 the diameter varies by 0.289 in and the packing height by 2.559 in. This means that as the gas flow doubles as shown in *figure 7*, the tower dimensions become larger, which implies an increase in the cost of packing and equipment construction material.

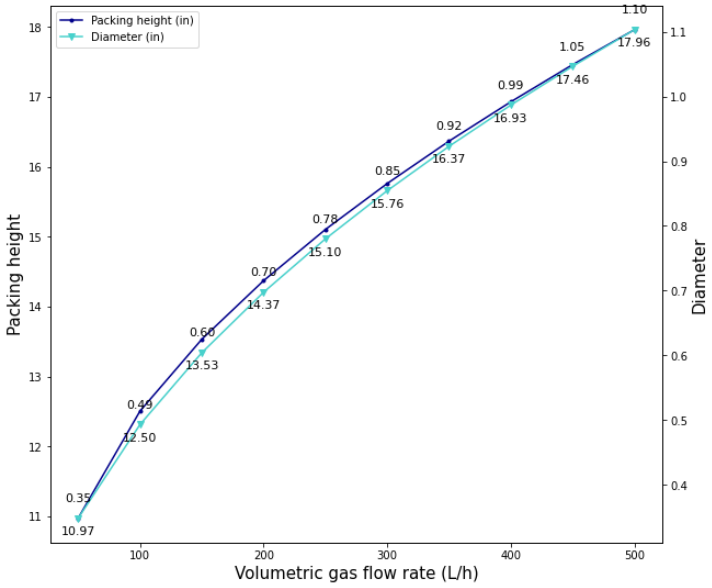

Figure 7*. Comparative graph of the diameter and height of the packing of an absorption tower with 80% CO_2 removal*

The design target for the packed absorption tower was set to achieve a CO_2 removal rate of 80% [19] as shown in *table 2*. By increasing the height of the packing, as can be seen in *figure 8*, the percentage of CO_2 removal presents a linear behavior while the height of the packing increases considerably. As can be seen in *figure 8*, in a CO_2 removal range of 0.1 to 0.8, the increase in pack height is not as significant, compared to a CO_2 removal range of 0.9 to 0.97 where the pack height increases considerably, which increases the associated equipment costs.

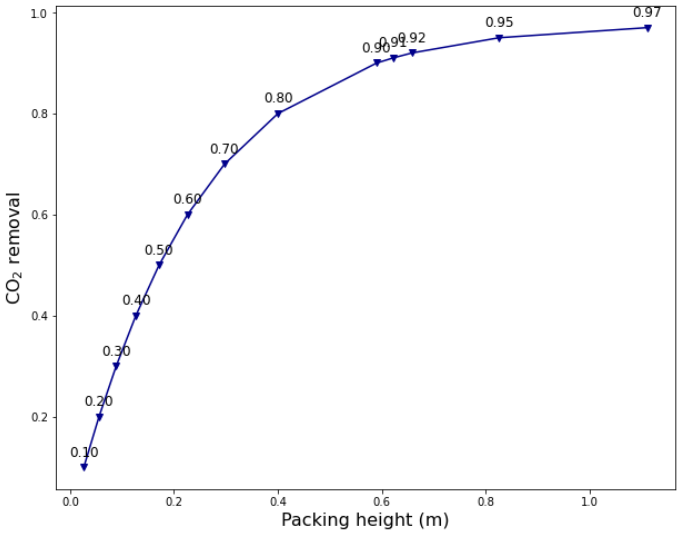

***Figure 8**. Graph that shows the behavior of the tower packing height with respect to the percentage of CO_2 removal.*

For an 80% CO_2 removal, different inlet concentrations were used to see the variation with respect to the packing height. As shown in *figure 9*, as the CO_2 input concentration increases, less packing material is needed, since CO_2 and aqueous amine have more contact area.

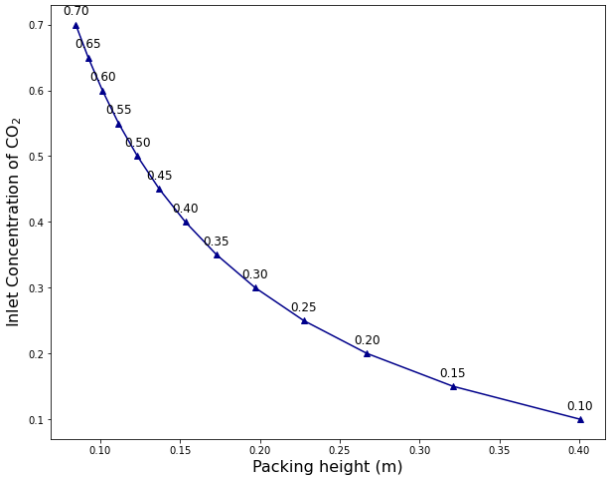

***Figure 9**. Graph that shows the behavior of the tower packing height with respect to lean loading (mol CO_2 / mol MEA)*

The velocity limit for the gas was 0.16 m/s, this value is important because it affects the resistance that will be encountered by the downflowing aqueous MEA and the pressure drop across the packing [26]. This value corresponds to a flooding percentage of 66%, which means that the aqueous MEA does not fill the entire column and the operation of the process is easier to carry out.

By performing the design in Python, it is possible to determine in a precise way all the parameters necessary for the calculation of the design such as: Column diameter, dimensionless numbers in the liquid and vapor phase, diffusion coefficient in the gas and liquid, mass transfer coefficients and packing height. Unlike Aspen Plus and Aspen HYSYS where these calculations are performed internally in the process.

Design of the absorption tower in Aspen Plus and Aspen HYSYS

As shown in *table 3*, similar results were obtained in Aspen Plus and Aspen HYSYS simulations. The most visible differences were the height of the tower packing and the percentage of flooding. These differences are attributed to the correlations for the liquid and vapor phases taken by each of the thermodynamic models, the correlations used for packing material in each of the simulators and the type of fixed parameters used in each simulator. The CO_2 removal percentage was established as an entry condition in both simulators and was specified as a fixed variable in Design Specs and Adjust manager of Aspen Plus and Aspen HYSYS, respectively.

Table 3. Results of the dimensions, mass flows, flood and pressure drop in the simulations of Aspen Plus and Aspen HYSYS

Parameter	Aspen Plus simulation	Aspen HYSYS simulation
Diameter (mm)	24.4	24.4
Packed height (mm)	1455	1200
Flooding (%)	50.68	45.58
Pressure drop (Pa/m)	379	375.2
CO_2 absorption (%)	80	80

According to the results, the Aspen HYSYS designed tower had a slightly lower pressure drop compared to Aspen Plus. However, both towers are within the established range of 200 to 400 Pa / m for pressure drop, which means that the gas and liquid flow rates used, and the properties of the Raschig ring packing prove to be good inlet conditions because the pressure drop remained in the range.

Both simulations have a flood percentage suitable for their operation, because when this percentage exceeds 80%, the solvent begins to accumulate and obstructs the cross-section resulting in increased pressure drops.

Even though Aspen Plus and Aspen HYSYS have been used in the simulation of absorption towers on a pilot scale and on an industrial scale [24,35,36] there is not much information in the open literature for the use of program correlations that facilitate obtaining data closer to the actual behavior of a laboratory scale tower. This means that the results obtained, although have been carried out with previously used methodologies, require an in-depth comparison. As can be seen in *figure 10*, which contains the packing heights with the respective removal percentage for Aspen Plus, Aspen HYSYS and Python simulations, when more CO_2 removal is required, a larger tower packing will be required. These values were obtained from the design of specifications of each simulator, where the concentration in the sweet gas outlet was varied from the concentration of CO_2 that entered the gas stream.

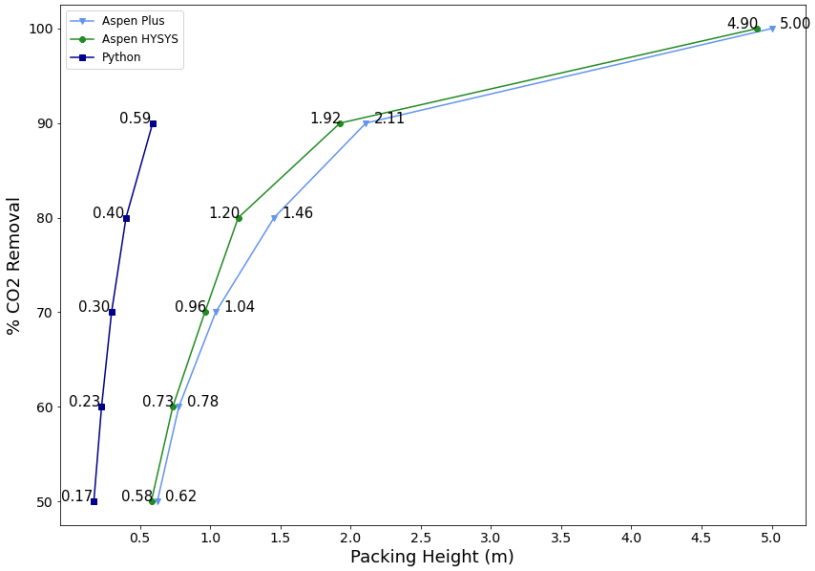

Figure 10. *CO_2 absorption at different packing heights of the absorption column in Aspen Plus, Aspen HYSYS and Python.*

A discrepancy in the data obtained in Python compared to Aspen Plus and Aspen HYSYS can be seen in *figure 10*. This is because Aspen Plus and Aspen HYSYS were simulated with a mixture of gases and the aqueous MEA as opposed to Python where a CO_2-MEA-WATER system was used. Therefore, in the two Aspen simulations, a larger surface area is needed which leads to a higher packing height.

This *figure 10* shows that, for CO_2 removal percentages greater than 88.33% and 91.04% in Aspen Plus and Aspen HYSYS respectively, the packing height increases over 2 meters. That is, to the point where the scale would no longer be considered laboratory scale. Unlike Python where CO_2 removal values greater than 80% do not exceed 1 meter, making it more suitable for a laboratory scale design.

Another important difference is that in Aspen HYSYS and Aspen Plus the inlet gas composition was assumed according to *table 1*, whereas for Python the inlet gas was assumed to be 10% CO_2 and 90% inert non-dissolved components. This affects the results in the design because the amount of CO_2 available to be absorbed by the amine is not the same, and the amount of amine that enters may be greater than that required for CO_2 removal, as can be seen in figure *11* of Aspen Plus.

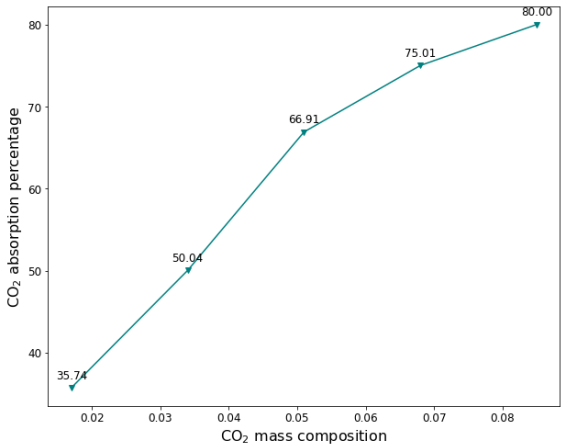

***Figure 11**. CO_2 absorption percentage vs initial CO_2 mass composition in the 1.455m Aspen Plus absorption tower*

As shown in *figure 11*, as the initial composition of CO_2 increases, the percentage of CO_2 absorption also increases. Therefore, due that in Aspen Plus and Aspen HYSYS simulations the CO_2 input was not the same as that used in Python, the CO_2 removal effort affected the results on the design dimensions, because as the CO_2 reacts, a greater effort of the system will be required, and it will be reflected in an increase in packing height as shown in *figure 10*. Therefore, the possibilities of obtaining the packing height of absorption tower with lower measures at 1m in the simulators were reduced, because this available CO_2 was lower from the beginning.

Finally, another difference in the simulations to which the discrepancies between the dimensions found are attributed is due the packing dimension type. Considering that Aspen Plus has the options of tower packing with dimensions greater than 13 mm, the fact that the simulator is commonly used for tower design larger than a laboratory scale is confirmed. Having used these Raschig rings with a size of 13 mm in the simulators, unlike Phyton where 10 mm ones were used, explains the increase in the height of the packing, because when these rings are larger, they reduce the cross-sectional flow area and therefore the height is increased, as shown in *figure 12.*

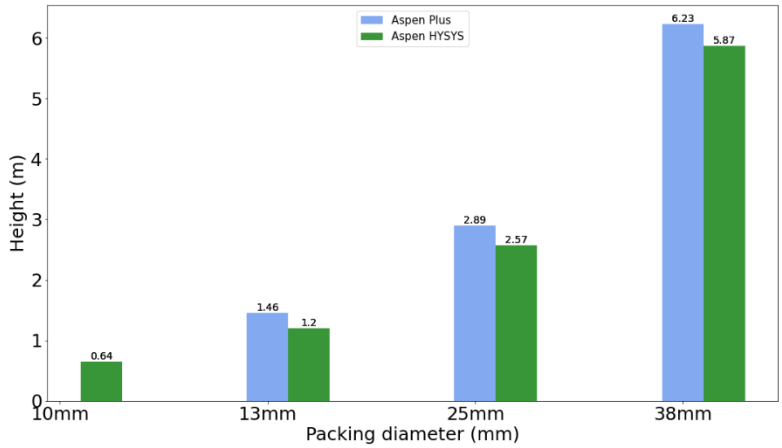

***Figure 12**. Tower packing height using the different sizes of Raschig Rings offered by the simulators to obtain 80% CO_2 absorption.*

As seen in *figure 12*, it is found that as a larger packing is used, the height of the packing will increase due to the reduction in the cross-sectional area of the tower. In addition, when using these larger packings, it is necessary that the diameter of the tower also increased because the packing size cannot be greater than this.

These results explain why the height of the simulated packings in Aspen Plus and Aspen HYSYS were greater than the height of the Python packing (0.40 m), because the size of the Raschig rings used was greater in the simulators (13mm) due to their availability within the program structure.

Mechanical design of the absorption tower

After performing the simulations in the programs mentioned above, the design of the absorption tower made in Python is chosen, since it yields dimensions of diameter and height of the package according to laboratory scale, achieving a removal of 80% of CO_2. For this reason, based on this simulation, a mechanical design of the equipment is made as shown in *table 4*.

Table 4. *Dimensions of the mechanical design*

Description	Results
D (m)	0.0217
H pack (m)	0.4
Packing type	Raschig rings
Liquid flow rate (m3/h)	0.006
Nominal packing size (mm)	10
Top size (m)	0.0747
Bottom size (m)	0.064
Pipes external diameters (m)	0.0213
Support thickness (m)	0.005
Pipe threaded couplings (lb/in2)	3000-6000
Thickness of threaded couplings (mm)	10
Hemispheric lid radius (m)	0.0107
Type of liquid distributor	Pipe-Arm

As shown in *table 4*, the pipes diameters are very close to the internal diameter of the tower, therefore, it was necessary to adapt the classic design of the absorption tower which has the outlet of the sweet gas in the lid of the tower and rich amine outlet just in the middle of the bottom, with the rich amine and sweet gas outlets on one side of the tower with horizontal outlets lines as seen in *figure 13*. Thus, no extra accessories like threaded couplings were required to join the tower and the pipes. The rich amine outlet pipe was located at the end of the tower so that no accumulation of liquid would be present, and the sweet gas outlet pipe was placed in such a way that the conventional design with a lid of the absorption tower was not affected in the top.

For this case, it was necessary to use a threaded coupling for the union between the packing section of the tower and the bottom of this, because the diameter of the tower was below the diameter required to use a flange.

Considering the height of the tower and the relation of the diameter of the tower and the diameter of the packing [37], it was not necessary to divide the package into several sections for the redistribution of the liquid. And considering the internal diameter of the tower (ID) and the liquid flow rate at the entrance of the tower [38], the liquid distributor that best matched these conditions was Pipe-Arm Model H1008. This is a spray nozzle distributor with the smallest liquid rate offered by the HMDS-process distributor.

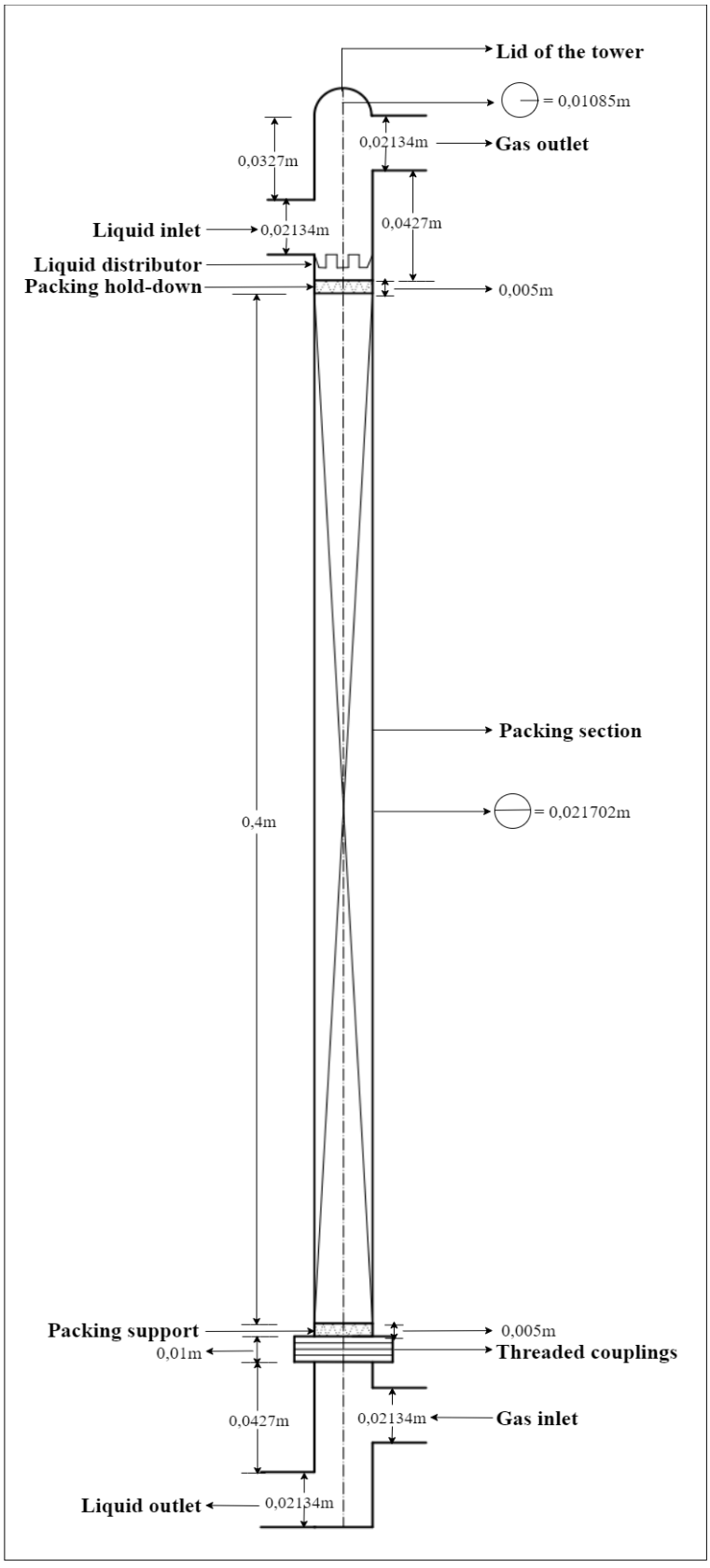

Figure 13. *Mechanical design of the absorption tower*

Having the dimensions of the packed absorption tower, an economic analysis of the construction of the equipment is carried out.

For this it is necessary to start from the cost of the packing (Raschig 10 mm ceramic rings), which is a function of the surface area and the supplier [33]. The value obtained is $ 7,529.23, this allows to fill all the available space in the height of the package and to achieve a better contact area.

Subsequently, to calculate the cost of the tower, the internal diameter obtained in Python of 0.8544 in (21.7017 mm) must be considered, as shown in *table 2*. Also, must be considered the total height of the equipment obtained from the mechanical design which has a value of 558.9 mm, the operating pressure of 125.6430 kPa and the stainless-steel 304 factor of 1.7. This gives an equipment cost of $916,710.01 and brings us to a capital expenditure (CAPEX) of $ 924,239.24.

In operating expenses, we must consider the cost of the pump and the purchase of the MEA, which gives us an annual OPEX of $135,123.00.

4. Conclusions

In this study, the design of a laboratory scale absorption tower was studied by using water and monoethanolamine as operating fluid. Therefore, a design strategy was implemented using different simulations for the design of the equipment were carried out in Aspen Plus, Aspen HYSYS and Python, to compare the results obtained in these programs. The Python simulation was developed with 80% CO_2 removal rate, thus obtaining a tower internal diameter of 21.7 mm and a packing height of 400.3 mm, this last parameter can change by varying the volumetric gas flow rate, the internal diameter of the tower, the percentage of carbon dioxide removal and / or the inlet concentration of CO_2 in the aqueous amine. With 80% of CO_2 removal, 2.0239 ton of CO_2 per year can be absorbed with this laboratory scale absorption tower.

The results obtained for the tower packing height in Aspen Plus and Aspen HYSYS were 1.455 m and 1.2 m respectively, and the diameter obtained for both simulators was 0.0244 m. These results show the dimensions of packing height and diameter were greater in Aspen Plus and Aspen HYSYS simulators than in Phyton because these flow simulators are better correlated to pilot and industrial scale unit operations, and because Raschig ring packing measure used in the simulators was 13 mm due that it was the smallest measure offered for this packing in Aspen Plus simulator unlike Python where 10 mm Raschig rings were used. This packing difference was shown to significantly increase tower packing height in simulators because as the packing is of greater measure, the cross – sectional area of the tower will be affected, and the system increases the height in response to this.

The Python design was chosen, which achieves 80% CO_2 removal, the dimensions obtained in this model are more in line with a laboratory scale plant and it is economically viable since it has a CAPEX of $ 924,239.24 and an OPEX of $135,123.00.

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